Supplementary Information

Synthesis and Structures of Transition Metal Pacman Complexes of Heteroditopic Schiff-Base Pyrrole Macrocycles

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Table 1: Crystallographic details

	j11001_H2LNMe(H2O)	jl9017_K2(LP)	lppd_Pd(LNMe)	Pd(LNMes)	j10095_Pd(LfNMe)
Crystal data					
Chemical formula	$C_{40}H_{37}N_5O_3$	$C_{35}H_{40}K_2N_4O_5(C_6H_6)_2$	$C_{32}H_{35}N_5O_2Pd$	$C_{43}H_{50}N_5O_2Pd$	$C_{40}H_{33}N_5O_2Pd$
M_r	635.75	831.13	628.05	775.28	722.11
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$
Temperature (K)	150	150	123	150	150
a, b, c (Å)	13.1353 (7), 14.794 (1), 18.6824 (13)	14.9201 (7), 20.8977 (11), 15.4577 (8)	9.7164 (9), 23.209 (2), 25.187 (3)	16.211 (6), 12.099 (4), 20.592 (7)	8.6736 (3), 14.6814 (4), 25.5451 (8)
α, β, γ (°)	68.452 (6), 80.755 (5), 82.839 (5)	90, 117.565 (2), 90	90, 91.066 (1), 90	90, 111.477 (5), 90	90, 97.840 (3), 90
V (Å^3)	3324.3 (4)	4272.5 (4)	5678.9 (10)	3758 (2)	3222.52 (17)
Z	4	4	8	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.08	0.27	0.69	0.54	0.62
Crystal size (mm)	0.58 × 0.25 × 0.18	0.42 × 0.29 × 0.19	0.2 × 0.2 × 0.2	0.12 × 0.05 × 0.02	0.1 × 0.09 × 0.03
Data collection					
Diffractometer	Agilent Technologies XCalibur	Bruker SMART APEXII	Rigaku Mercury diffractometer	Rigaku Saturn70 diffractometer	Agilent Technologies XCalibur
Absorption correction	Multi-scan *CrysAlisPRO*	Multi-scan *SADABS*	Multi-scan	Multi-scan	Multi-scan *CrysAlisPRO*
T_{min}, T_{max}	0.902, 1.000	0.643, 0.745	0.805, 1.000	0.873, 1.000	0.747, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	57357, 14984, 10735	42106, 8764, 7237	43926, 15119, 12143	36963, 6873, 6133	29081, 7284, 6001
R_{int}	0.037	0.043	0.030	0.096	0.057
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.649	0.626	0.714	0.603	0.650
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.132, 1.02	0.072, 0.185, 1.10	0.049, 0.130, 1.11	0.057, 0.148, 1.08	0.044, 0.102, 1.08
No. of reflections	14984	8764	15119	6873	7284
No. of parameters	867	519	727	468	434
No. of restraints	0	3	0	36	0

H-atom treatment	Riding	Riding	Riding	Riding	Riding
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.55, -0.25	0.88, -0.47	2.52, -0.64	2.07, -0.88	1.00, -0.83
CCDC	895814	895815	895816	895817	895818

	j10084cold_TiCl(Lp)	jl9054_VClH2OLp	CrClH2OLfNMe	j10088a_CoH2OOHLfP	j12003_Co(H2O)(LfNMe)	jl0042_Co(LMes)
Crystal data						
Chemical formula	$C_0C_{39}H_{48}ClN_4O_6Ti$	$C_{35}H_{42}ClN_4O_6V$	$C_{46}H_{39}ClCrN_5O_3$	$C_{43}H_{38}CoN_4O_8$	$C_{40}H_{35}CoN_5O_3\cdot C_6H_6$	$C_{43}H_{50}CoN_5O_2$
M_r	752.16	701.12	797.27	797.70	770.77	727.81
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	150	150	120	150	170	100
a, *b*, *c* (Å)	13.540 (5), 20.124 (5), 14.798 (5)	9.9312 (3), 16.3385 (4), 21.0755 (5)	12.9879 (10), 21.2422 (17), 14.5019 (8)	13.8243 (9), 24.612 (3), 15.1874 (10)	15.0941 (2), 17.0962 (2), 14.9472 (2)	16.3981 (6), 11.9955 (3), 20.8155 (8)
α, β, γ (°)	90.000 (5), 111.333 (5), 90.000 (5)	90, 99.777 (1), 90	90, 104.939 (7), 90	90, 100.065 (6), 90	90, 104.537 (2), 90	90, 113.323 (5), 90
V (Å^3)	3756 (2)	3370.06 (15)	3865.7 (5)	5087.9 (7)	3733.67 (8)	3759.9 (2)
Z	4	4	4	4	4	4
Radiation type	Mo *K*α	Mo *K*α	Cu *K*α	Mo *K*α	Mo *K*α	Cu *K*α
μ (mm^{-1})	0.35	0.43	3.46	0.38	0.51	3.91
Crystal size (mm)	0.08 × 0.07 × 0.04	0.26 × 0.20 × 0.16	0.12 × 0.08 × 0.05	0.09 × 0.03 × 0.03	0.60 × 0.44 × 0.22	0.51 × 0.15 × 0.10
Data collection						
Diffractometer	Xcalibur, Eos diffractometer	Bruker Smart Apex CCD diffractometer	SuperNova, Dual, Cu at zero, Atlas diffractometer	Xcalibur, Eos diffractometer	Xcalibur, Eos diffractometer	SuperNova, Dual, Cu at zero, Atlas diffractometer
Absorption correction	Multi-scan *CrysAlis PRO*	Multi-scan *SADABS* 2007/2	Gaussian *CrysAlis PRO*	Multi-scan *CrysAlis PRO*	Multi-scan *CrysAlis PRO*	Multi-scan
T_{min}, T_{max}	0.988, 1.000	0.662, 0.745	0.784, 0.882	0.710, 1.000	0.887, 1.000	0.409, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24594, 8341, 3571	6891, 6891, 1414	28054, 4277, 2771	43497, 12094, 5264	41617, 7918, 6915	34244, 7461, 6142
R_{int}	0.031	0.057	0.106	0.094	0.026	0.071
θ_{max} (°)	27.5	26.4	51.9	29.3	26.7	73.3
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.626	0.510	0.688	0.633	0.621
Refinement						
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.053, 0.146, 0.82	0.041, 0.112, 0.78	0.094, 0.301, 1.10	0.129, 0.393, 1.13	0.035, 0.094, 1.06	0.052, 0.142, 1.04
No. of reflections	8341	6891	4277	12094	7918	7461
No. of parameters	462	434	506	505	503	466
No. of restraints	0	3	0	0	2	0
H-atom treatment	Riding	Riding	H-atom parameters	Riding	H atoms treated by a	Riding

			constrained		mixture of independent and constrained refinement	
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.59, -0.44	0.53, -2.29	1.18, -0.68	1.34, -1.40	0.35, -0.50	0.60, -0.45
CCDC	895819	895820	895821	895822	895823	895824

	Fe2(2+2LP)	jl0024_Mn2(2+2LP)	jl0035_Co(2+2LNMe)
Chemical formula	$C_{73}H_{83}Fe_2N_8O_{10}$	$C_{70}H_{79}Mn_2N_8O_{10}$	$C_{64}H_{70}Co_2N_{10}O_4$
M_r	1344.17	1302.29	1161.16
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$	Orthorhombic, *Pccn*
Temperature (K)	150	150	100
a, *b*, *c* (Å)	12.120 (3), 13.077 (3), 20.726 (5)	25.365 (5), 12.448 (5), 20.697 (5)	12.4047 (1), 18.6551 (2), 24.0651 (3)
α, β, γ (°)	95.077 (8), 90.782 (6), 95.088 (11)	90.000 (5), 105.979 (5), 90.000 (5)	90, 90, 90
V (Å^3)	3258.4 (14)	6282 (3)	5568.93 (10)
Z	2	4	4
Radiation type	Mo *K*α	Cu *K*α	Cu *K*α
μ (mm^{-1})	0.51	3.82	5.14
Crystal size (mm)	0.10 × 0.10 × 0.03	0.22 × 0.15 × 0.07	0.1 × 0.07 × 0.05
Diffractometer	Rigaku Mercury diffractometer	Agilent Technologies SuperNova	Agilent Technologies SuperNova
Absorption correction	Multi-scan	Multi-scan *CrysAlis PRO*.	Multi-scan *CrysAlis PRO*.
T_{min}, T_{max}	0.368, 1.000	0.884, 1.000	0.609, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20681, 11277, 8773	60916, 12465, 9643	27037, 5502, 4591
R_{int}	0.070	0.046	0.059
(sin θ/λ)$_{max}$ (Å^{-1})	0.602	0.622	0.621
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.083, 0.249, 1.04	0.033, 0.086, 0.85	0.045, 0.125, 1.03
No. of reflections	11277	12465	5502
No. of parameters	842	811	364
No. of restraints	24	0	0
H-atom treatment	Riding	Riding	Riding
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	1.13, -1.06	0.71, -0.23	0.46, -0.43
CCDC	895825	895826	895827

Computer programs: *CrysAlis PRO (*Agilent Technologies, 2011); *SMART* (Bruker, 2007), *CrystalClear*-SM

Expert 2.0 rc13 (Rigaku, 2009), *SAINT* (Bruker, 2007), *CrystalClear* (Rigaku Inc., 2007), *SORTAV* (Blessing, 1995), *SIR92* (Giacovazzo *et al.*, 1993), SUPERFLIP (Palatinus & Chapuis, 2007), *SHELXS/L97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 1997), *enCIFer* (Allen *et al.*, 2004), *WinGX* publication routines (Farrugia, 1999)

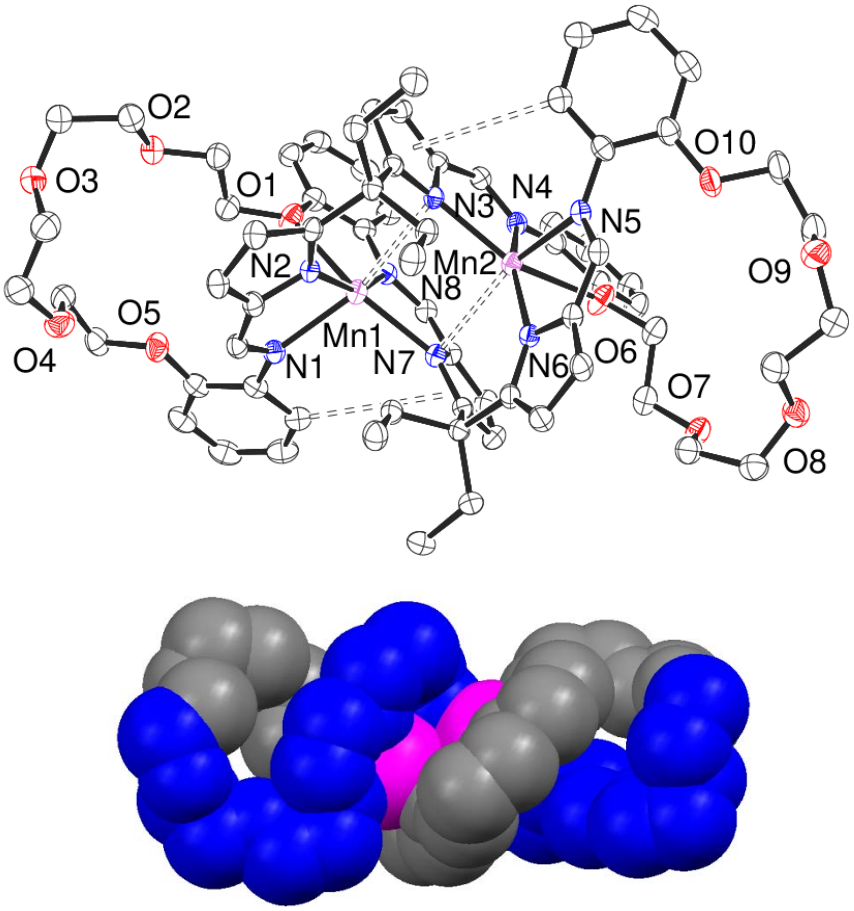

Figure S1: X-ray crystal structure of $Mn_2(^{2+2}L^{P})$. For clarity, all hydrogen atoms and solvent of crystallisation are omitted (displacement ellipsoids are drawn at 50% probability).